checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: apx2108

```
Bond precision:  C-C = 0.0148 A          Wavelength=0.71073

Cell:             a=16.436(4)      b=18.645(5)      c=19.723(5)
                  alpha=90         beta=90          gamma=90
Temperature:      140 K
```

	Calculated	Reported
Volume	6044(3)	6044(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	?
Moiety formula	C32 H47 Br O U	?
Sum formula	C32 H47 Br O U	C32 H47 Br O U
Mr	765.63	765.64
Dx,g cm-3	1.683	1.683
Z	8	8
Mu (mm-1)	6.715	6.715
F000	2992.0	2992.0
F000’	2914.30	
h,k,lmax	20,22,24	20,22,24
Nref	11639[6392]	11618
Tmin,Tmax	0.286,0.818	0.296,0.824
Tmin’	0.192	

```
Correction method= # Reported T Limits: Tmin=0.296 Tmax=0.824
AbsCorr = MULTI-SCAN

Data completeness= 1.82/1.00      Theta(max)= 25.810

R(reflections)= 0.0416( 9002)     wR2(reflections)= 0.1004( 11618)

S = 0.991                 Npar= 660
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
STRVA01_ALERT_4_C           Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.416
          From the CIF: _refine_ls_abs_structure_Flack_su    0.010
PLAT213_ALERT_2_C Atom C41            has ADP max/min Ratio .....        4.0 prolat
PLAT213_ALERT_2_C Atom C51            has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C53            has ADP max/min Ratio .....        3.3 prolat
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range       3.6 Ratio
PLAT222_ALERT_3_C Large Non-Solvent  H     Uiso(max)/Uiso(min) ...       4.4 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C5     --  C10     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C43    --  C47     ..       0.18 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01477 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF      Please Do !
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.416 Note
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  U2     --  Br2     ..        5.2 s.u.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C8 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C51 Check
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 19/11/2015; check.def file version of 17/11/2015

Datablock apx2108 - ellipsoid plot